

Fermions with attractive interactions on optical lattices and implications for correlated systems

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In this paper we address the behavior of the superfluid transition temperature T_c in the attractive Hubbard model. The attractive Hubbard model can be regarded as the generalization of BCS to Bose Einstein condensation (BEC) crossover to a lattice and as such, may have implications for future optical lattice studies. Nevertheless, the BEC limit of the Hubbard model is very different from that of the more well studied Fermi gases, owing to the strong inter-site repulsion between pairs. Here we address systematically the effects of pairing fluctuations for all filling fractions over the entire range of attractive interaction strength. A central conclusion of our work is that in a lattice, around half filling, the smooth evolution from the BCS to the BEC limits is interrupted: T_c vanishes when the system approaches the bosonic regime with increasing interaction strength. We suggest that this interruption of crossover may signal a quantum critical transition to another form of superfluid not continuously connected to a BCS-like phase. A simple variational ansatz for an alternate ground state in this more strongly coupled superfluid is presented. A generalization of the (s -wave) Hubbard model to d -wave pairing allows us to address issues of relevance to high T_c superconductivity. The phase diagram (representing the pairing or pseudogap onset temperature T^* and T_c) shows that here too, one observes a vanishing of T_c when T^* becomes sufficiently large. Given this predicted breakdown of the crossover, and given the striking similarity to features of the cuprate phase diagram, we suggest that future experiments on ultracold fermions in optical lattices should not be exclusively limited to the repulsive Hubbard model, but should address the attractive model in order to elucidate features of high temperature superconductivity.

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I. INTRODUCTION

Recent experiments on ultracold Fermi gases of ^{40}K [1] and ^6Li [2] in the presence of an optical lattice are creating considerable interest in the community. These experiments can be viewed as quantum simulations [3, 4] of important condensed matter problems such as the repulsive and attractive fermion Hubbard models. In these experiments one can vary (albeit, not independently) both the on-site interaction strength between fermions and the lattice depth and in this way change the interaction U and hopping t . In the case of *attractive* interaction U , one can view the Hubbard model as generalizing the important problem of BCS–Bose-Einstein condensation (BEC) crossover [5, 6, 7] to the case of a lattice. This crossover study represents an exciting research area because it provides a means of extending what is arguably the paradigm of all theories in condensed matter physics (BCS theory) to a far more general situation.

Many have argued that [8] the key to high temperature superconductivity comes from the *repulsive* Hubbard model and there is a growing impetus to use cold atoms to address the issue of whether this repulsive model can ultimately lead to d wave superconductivity [9, 10]. Nevertheless, our paper is based on the premise that we have potentially as much to learn about high T_c superconductors from the attractive as from the repulsive Hubbard case. This attractive model represents a generalization of BCS-BEC crossover which is of current interest in atomic Fermi systems [11, 12] to now include the presence of an optical lattice. We will, in addition to the s -wave case, consider a natural generalization to the d -

wave pairing symmetry. The former, however, has been more extensively addressed in the literature and is of considerable value since the experimental counterpart is more straightforward. The latter is more relevant to high T_c superconductors.

We note that the BCS-BEC crossover scenario is argued [13] to be relevant to high temperature superconductors because of their anomalously short coherence length. Additional support for the potential relevance of the attractive Hubbard model (AHM) to the copper oxides comes from the fact that this crossover scenario naturally leads to a “pseudogap” phase which is quite prominent in the cuprates, although there is still no consensus on its origin. [8, 11, 14] The pseudogap state corresponds to a regime (above T_c) where there is a gap for exciting fermionic quasi-particles. Within the crossover scenario a natural interpretation of this gap associates it with the existence of metastable (sometimes called pre-formed) pairs arising from the stronger-than-BCS attractive interaction. These noncondensed pairs require an added energy in order to break them apart and create fermionic excitations.

A central goal of this paper is to present a phase diagram for the various regions of d - and s -wave superfluid stability as a function of interaction strength and band filling. In this context, we also present a phase diagram indicating how the characteristic temperatures, i.e., the pseudogap onset temperature T^* and the condensation temperature T_c , vary with the strength of the attractive interaction in the d -wave case. When the attraction gets progressively stronger (as measured by the size of T^*), T_c begins to decrease and ultimately vanishes. This behavior is strikingly similar to that found in the cuprate phase diagram ([8], especially Fig. 7) where, via larger T^* , one can associate stronger attraction with reduced doping concentration. These observations suggest that future cold gas experiments should not focus solely on the repulsive Hubbard

model, but also give extensive attention to the attractive case.

In so far as they relate to the high temperature superconductors, the attractive and repulsive Hubbard models should be directly compared. In particular, these two models may be essentially equivalent if in the attractive case, the interaction is presumed to be d -wave. The repulsive Hubbard model is thought to give rise to a d -wave pairing [8, 9, 10] although this has yet to be conclusively demonstrated. Given that the pairing symmetry in the cuprates is known to be d -wave and that the pair size is anomalously small, it is certainly of equal interest to study a d -wave generalization of the *attractive* Hubbard model, as we do here. Within this latter context no assumption is made about the microscopic origin of the attractive interaction. Quite possibly, however, this inter-site attraction comes the Coulomb interaction which is repulsive at short distances, but can be even more complex than contemplated [15, 16] by the simple repulsive Hubbard model.

While there have been a number of numerical studies of the s -wave pairing model [17, 18, 19], along with approaches based on dynamical mean field theory [20, 21, 22, 23], ours is the only systematic study over all filling fractions and over the entire range of attractive interactions. We investigate the stability of the BCS-Leggett like ground state (applied to the lattice). This state is a natural one to consider for the purposes of ultimately shedding light on the cuprates, since there is a strong belief in the community [8, 11, 14] that when superconductivity is present, it is in many aspects not so different from the d -wave BCS state. In this way we argue that, while more sophisticated ground state wave functions might be of great interest for reaching a general understanding, they may not be of specific relevance to the cuprates.

We find that, even though the strict $T = 0$ mean-field equations suggest that superfluidity can occur everywhere, fluctuation effects lead to a vanishing T_c over an extended range sufficiently near half filling and for moderately strong attraction. An important clue underlying this breakdown of BCS-BEC crossover is that it occurs very close to the point where the fermionic chemical potential μ changes sign. We naturally interpret the $\mu = 0$ point as corresponding to the transition into a regime where the system is effectively bosonic. Here the “bosons” are associated with condensed or noncondensed (finite momentum) Cooper pairs.

To gain further insight, we are motivated, then, to consider an *effective* bosonic model representing the AHM. Indeed, when one expands this Hamiltonian in terms of $t^2/|U|$ the model which emerges contains bosonic hopping as well as an inter-site repulsion of precisely the same magnitude. At low density the repulsion is not important, and the system is expected to support BCS-like superfluidity with a T_c of order $t^2/|U|$, as originally conjectured in the important paper by Nozieres and Schmitt-Rink (NSR) [6]. However, closer to half filling in the t^2/U -expanded bosonic Hamiltonian the inter-boson interactions are *strong*. We emphasize that in this simple BCS-Leggett ground state the interaction between bosons is implicitly taken to be weak. More sophisticated wave functions are required to capture the effects of stronger inter-boson interactions [24] which must go even beyond Bogoliubov level theory to be consistent with the physics

of the t^2/U -expanded Hubbard model. This, then, provides an explanation for the failure of this simple BCS trial wave function to support a superfluid phase in the BEC regime on a lattice. Finally, these studies are extended to the d -wave case as well, where the breakdown of the BCS-Leggett like superfluid occurs well before the chemical potential becomes negative.

There has been a substantial literature on BCS-BEC crossover on the subject of Fermi gases [11, 12, 14] with tunable attractive interactions. There is also considerable interest in whether an analogous crossover can be observed for fermions on a lattice [25, 26]. To effect this crossover we note that there are two ways of increasing the dimensionless attraction U/t , either by changing the lattice depth or changing the on-site attraction U by exploiting a Feshbach resonance. For the present purposes of addressing BCS-BEC crossover in the context of the AHM [4, 27] (which we have argued above may contain information about high temperature superconductors) we should not exploit these Feshbach effects. Rather, the hopping t and the on-site attraction U are varied by changing parameters of the optical lattice. Thus, our conclusions about the interruption of BCS-BEC crossover near the onset of BEC are entirely associated with the Hubbard model and do not pertain if one uses a Feshbach resonance to create bosonic degrees of freedom, prior to applying an optical lattice. In this alternative circumstance the more appropriate many body model is the Bose Hubbard model which we do not consider here.

There is an extensive literature which addresses the AHM, ([28] and references therein), principally in the two-dimensional case because of associations with high-temperature superconductivity. In a related fashion, the possibility of observing (bosonic-like) Mott insulating states at full filling has been the motivation for studies from a number of groups [29, 30, 31, 32], particularly from the atomic physics community. There has also been a focus on charge density wave states which are energetically degenerate with the superfluid phase at precisely half filling and may compete or co-exist with superfluidity [28, 33] slightly away. Indeed, a supersolid phase contemplated in this literature is viewed as a mixture of charge density wave and superfluidity. Finally, we note that there is also a methodology for addressing the AHM via a mapping to the repulsive Hubbard case. Except at exactly 1/2 filling, the counterpart repulsive model must be solved in the presence of a rather complicated constraint, which is difficult to implement. A general theorem which states that, in the AHM, the ground state contains no magnetic order [34], must be imposed [28] in any study based on this mapping.

For the most part these previous studies have been at zero temperature. Here we focus on general temperatures, T . By choosing to address the superfluid transition temperature, T_c , we effectively introduce fluctuation contributions in a fashion that is consistent with the BCS-Leggett ground state and capable of addressing finite temperatures. Without these fluctuations, in the s -wave case, it appears that a BCS-Leggett superfluid ground state is stable for all parameters. By considering the entire range of (attractive) interaction strengths and filling factors, we enter into regimes which have also not

been addressed by complementary numerical or mean field techniques.

Our theoretical scheme is based on a particular T -matrix approximation for the pairing fluctuations which is compatible with this simplest ground state. Alternative T -matrix schemes have been applied to attractive Hubbard models in a number of different variations. The transition temperature T_c was estimated in [17] within an approach in which there is no pseudogap phase in the normal state. By contrast, here as in earlier work [25, 35, 36], we use a scheme in which superconductivity emerges in the presence of a pseudogap. Alternative approaches based on dynamical mean field theory [20, 21, 22] in three dimensions (3D) and on quantum Monte Carlo simulations in 3D [18] or in 2D [19] have also addressed the size of the transition temperature. For intermediate attraction strengths, a maximum in the T_c curves is found, which some have argued [26, 27] corresponds to the regime where BCS-BEC crossover occurs. However, we stress that this maximum appears deep in the fermionic regime, quite far from where the fermionic chemical potential μ becomes negative.

It should be noted that there are also extensive studies of the Bose Hubbard model [37, 38, 39] which are viewed as relevant to the strongly attractive regimes of the fermion AHM. We emphasize here, however, that there is an important distinction between the composite boson BEC limit and the Bose Hubbard model, due to the different commutation properties of the field operators for fermion pairs versus those for true bosons. This difference is less important in the very low filling regime, but it cannot in general be ignored. Finally, on the subject of BCS-BEC crossover for the d -wave case, there are earlier studies [35, 40] in the literature. In Ref. [40] a simplified model addressed the 2D square lattice at $T = 0$.

II. GENERAL FORMALISM: BCS-BEC CROSSOVER ON A LATTICE

The AHM Hamiltonian is given by

$$H^{\text{AHM}} = \sum_{\langle i,j \rangle, \sigma} t_{ij} c_{i\sigma}^\dagger c_{j\sigma} + \frac{1}{2} U \sum_i (n_i - 1)^2. \quad (1)$$

Here $\langle i, j \rangle$ denotes nearest neighbors, t_{ij} denotes the hopping coefficient, $\sigma = \uparrow, \downarrow$ denotes spins, $U < 0$ is the on-site attractive coupling constant, $n_i = n_{i\uparrow} + n_{i\downarrow}$, and $n_{i\sigma} = c_{i\sigma}^\dagger c_{i\sigma}$. We consider the case where there is an equal population of both fermion spin states. The fermion filling factor is $n = \sum_i \langle n_i \rangle / N$, where N is the total number of sites on the lattice. In the single-band tight-binding approximation only the case $0 < n < 1$ needs to be considered due to particle-hole symmetry.

In order to include d -wave pairing as well, it is convenient to consider a generalization of the AHM in a momentum space representation.

$$H - \mu \hat{N} = \sum_{\mathbf{k}\sigma} \xi_{\mathbf{k}} c_{\mathbf{k}\sigma}^\dagger c_{\mathbf{k}\sigma} + \sum_{\mathbf{k}\mathbf{k}'\mathbf{q}} V_{\mathbf{k},\mathbf{k}'} c_{\mathbf{k}+\mathbf{q}/2\uparrow}^\dagger c_{-\mathbf{k}+\mathbf{q}/2\downarrow}^\dagger c_{-\mathbf{k}'+\mathbf{q}/2\downarrow} c_{\mathbf{k}'+\mathbf{q}/2\uparrow}. \quad (2)$$

Here $\xi_{\mathbf{k}} = \epsilon_{\mathbf{k}} - \mu$, μ is the fermion chemical potential, $\hat{N} = \sum_{\mathbf{k}} c_{\mathbf{k}}^\dagger c_{\mathbf{k}}$ is the total number operator, $\epsilon_{\mathbf{k}}$ is the energy in the tight-binding band. The interaction in momentum space assumes the separable form $V_{\mathbf{k},\mathbf{k}'} = U_\alpha \varphi_{\mathbf{k}} \varphi_{\mathbf{k}'}$. Here $U_\alpha = U$ and $\varphi_{\mathbf{k}} = 1$ for s -wave and $U_\alpha = U_d$ and $\varphi_{\mathbf{k}} = \cos k_x - \cos k_y$ for d -wave pairing. For the s -wave case, we consider isotropic 3D square lattices with $\epsilon_{\mathbf{k}} = 2t(3 - \cos k_x - \cos k_y - \cos k_z)$, where t , the hopping integral, serves as the unit of energy. For d -wave pairing we consider quasi-2D square lattices with $\epsilon_{\mathbf{k}} = 2t_{\parallel}(2 - \cos k_x - \cos k_y) + 2t_{\perp}(1 - \cos k_z)$, where t_{\parallel} and t_{\perp} are the in-plane and out-of-plane hopping integrals, respectively. We use t_{\parallel} as the unit of energy, and presume, for definiteness, an anisotropic ratio $t_{\perp}/t_{\parallel} = 0.01$, which is reasonable for the cuprate superconductors [35].

When the attraction is weak ($|U_\alpha|/t \rightarrow 0$), the superfluid phase consists of loosely bound pairs, as in a BCS model. As $|U_\alpha|$ is progressively increased the pairs become more tightly bound and the system crosses over over to a BEC-based description in which there are composite bosons confined to a lattice. The simplest possible ground state for describing this crossover on a lattice is that associated with BCS-Leggett theory [5]. We will adopt this ground state here:

$$|BCS\rangle = \prod_{\mathbf{k}} (u_{\mathbf{k}} + v_{\mathbf{k}} c_{\mathbf{k}\uparrow}^\dagger c_{-\mathbf{k}\downarrow}) |0\rangle. \quad (3)$$

Here the coefficients $u_{\mathbf{k}}^2, v_{\mathbf{k}}^2 = (1 \pm \xi_{\mathbf{k}}/E_{\mathbf{k}})/2$ and the quasi-particle dispersion $E_{\mathbf{k}} = \sqrt{\xi_{\mathbf{k}}^2 + \Delta^2 \varphi_{\mathbf{k}}^2}$. This ground state presumes that the condensation is complete and is, more generally, appropriate only for weakly interacting bosons or Cooper pairs. In the single trap experiments the BEC asymptote is indeed associated with free bosons and one might expect this wave function to be a reasonable starting point. On the lattice, in the BEC limit, however, the repulsive interaction is equal to the effective kinetic energy of the pairs (as will be discussed below). Therefore, in a properly self-consistent theory, one might expect to see a break down of this ansatz for the ground state wave function near half filling where the effects of inter-pair repulsion are no longer negligible.

A. Present T-matrix Scheme

To solve for T_c in a fashion consistent with the known ground state constraints [5, 6] of the gap and fermion number equations, we follow earlier calculations [11, 14, 25], based on a T -matrix theory for pairing fluctuations. The T -matrix is given by $t(K, K', Q) = t(Q) \varphi_{\mathbf{k}} \varphi_{\mathbf{k}'}$, and contains two contributions, $t(Q) = t_{sc}(Q) + t_{pg}(Q)$, describing the condensed and noncondensed pairs, respectively. Here we take $K \equiv (i\omega_n, \mathbf{k})$, $K' \equiv (i\omega_{n'}, \mathbf{k}')$, and $Q \equiv (i\Omega_m, \mathbf{q})$ as four-vectors. We use ω_n and Ω_m to represent the Matsubara frequencies for fermions and bosons, respectively, and $\sum_K \equiv T \sum_{\omega_n} \sum_{\mathbf{k}}$. It can be shown that if one takes $t_{sc}(Q) = -(\Delta_{sc}^2/T) \delta(Q)$, as $T \rightarrow 0$ the T -matrix theory is consistent with the constraints in the BCS-Leggett ground state. Here Δ_{sc} is the order parameter which vanishes at T_c .

but is equal to the total gap at $T = 0$. The contribution from the noncondensed pairs, which contains the sum of particle-particle scattering ladder diagrams, is

$$t_{pg}(Q) = \frac{U_\alpha}{1 + U_\alpha \chi(Q)}, \quad (4)$$

and the pair susceptibility is $\chi(Q) = \sum_{\mathbf{k}} G(K) G_0(Q - K) \varphi_{\mathbf{k}-\mathbf{q}/2}^2$. Here $G_0(K) = (i\omega_n - \xi_{\mathbf{k}})^{-1}$ is the bare Green's function and $G(K)$ is its dressed counterpart.

To define the appropriate dressed Greens functions, we adopt the usual T -matrix expression for the fermion self-energy given by $\Sigma(K) = G_0^{-1}(K) - G^{-1}(K) = \sum_Q t(Q) G_0(Q - K) \varphi_{\mathbf{k}-\mathbf{q}/2}^2$. This self-energy can be approximated as $\Sigma(K) = -\Delta^2 G_0(-K) \varphi_{\mathbf{k}}^2$, where $\Delta^2 = \Delta_{sc}^2 + \Delta_{pg}^2$ and the pseudogap contribution is

$$\Delta_{pg}^2 \equiv - \sum_Q t_{pg}(Q) \quad (5)$$

The total fermion number equation is given by $n = 2 \sum_K G(K)$, or

$$n = \sum_{\mathbf{k}} \left[\left(1 - \frac{\xi_{\mathbf{k}}}{E_{\mathbf{k}}} \right) + 2f(E_{\mathbf{k}}) \left(\frac{\xi_{\mathbf{k}}}{E_{\mathbf{k}}} \right) \right]. \quad (6)$$

The BEC condition requires that the pairs have zero chemical potential at and below T_c : $t_{pg}^{-1}(0) = U_\alpha^{-1} + \chi(0) = 0$, i.e.,

$$t_{pg}^{-1}(0) = U_\alpha^{-1} + \sum_{\mathbf{k}} \frac{1 - 2f(E_{\mathbf{k}})}{2E_{\mathbf{k}}} \varphi_{\mathbf{k}}^2 = 0, \quad T \leq T_c. \quad (7)$$

For $T \leq T_c$, to satisfy this BCS-like gap equation (which naturally emerges for Δ within the present T -matrix scheme), Δ must necessarily contain a contribution from both a non-zero superfluid order parameter, Δ_{sc} , and a contribution associated with noncondensed pairs, Δ_{pg} . In this way and in the weak coupling limit, this approach represents a re-interpretation of BCS theory which underlines the strong similarity to the treatment of ideal gas BEC. The contribution from noncondensed pairs enters through a gap equation, not a number equation, however. The transition temperature T_c is the temperature above which Δ_{sc} vanishes and is determined by solving Eqs. (5), (6), and (7) self-consistently.

Below T_c the T -matrix may be expanded as $t_{pg}^{-1} \approx a_1 \Omega^2 + a_0 \Omega - \xi^2 q^2 + i\Gamma_{\mathbf{q}}$ after analytic continuation. This simplifies the evaluation of Eq. (5). The effect of the $a_1 \Omega^2$ term can be neglected except in a narrow regime near half filling, where particle-hole symmetry leads to $a_0 \rightarrow 0$. The contribution of pairs is dominated by those near the bottom of their energy band so the dispersion is further approximated as $\Omega_{\mathbf{q}} = \xi^2 q^2 / a_0 = q^2 / 2M_p$, where M_p is the effective mass of the pairs on a lattice. Note that $\Gamma_{\mathbf{q}} \ll \xi^2 q^2$ in the long wavelength limit so that it is set to 0 in our numerical calculations.

B. The strong attraction limit

For the case of s -wave pairing, it is useful at this stage to study an approximated Hamiltonian in the limit that $|U|/t$ is

finite but very large so that the hopping term can be treated as a perturbation. Following Refs. [41, 42] and dropping overall constants, the Hamiltonian can be rewritten as

$$H_{eff} = - \sum_{\langle i,j \rangle} J b_i^\dagger b_j + \sum_{\langle i,j \rangle} J n_{b_i} n_{b_j}. \quad (8)$$

Here $J = 2t^2/|U|$, $b_i = c_{i\downarrow} c_{i\uparrow}$, $b_i^\dagger = c_{i\uparrow}^\dagger c_{i\downarrow}^\dagger$, and $n_{b_i} = b_i^\dagger b_i$. The pair operators b_i and b_i^\dagger are not strictly boson annihilation and creation operators, since their commutator $[b_i, b_i^\dagger] = 1 - n_i$, and $\{b_i, b_i\} = 0$, where n_i represents the number of fermions at site i . The Pauli principle insures that these “bosons” are hard core bosons. This effective Hamiltonian is equivalent to an XXZ magnetic model with an effective external field in the z direction; here the average magnetization must have a fixed value equal to $(n - 1)/2$ (see [28]).

It is important to stress that Eq. (8) contains a nearest neighbor inter-site repulsion which is of the same value J as the boson hopping term. This inter-site repulsion becomes progressively more important when the fermion filling is close to one half. While the fact that the kinetic energy in Eq. (8) varies as t^2/U is relatively straightforward to understand, the origin of the inter-site repulsion is more subtle. This term arises [6] from the energy lowering associated with virtual hopping of fermions. Clearly the Pauli principle leads to a constrained hopping; if a pair has an occupied nearest neighbor site, then hopping will be suppressed, thereby raising the energy. In this way we see that there is an effective inter-site repulsion between the pairs.

The Hamiltonian of Eq. (8) should be contrasted with the boson Hubbard model (BHM) which has been widely studied [37] in the context of the Mott insulator-superfluid transition. The BHM corresponds to true bosons on a lattice, where the kinetic energy contribution and the *on-site* repulsion U_B can be varied independently:

$$H^{BHM} = - \sum_{\langle i,j \rangle} J_B \bar{b}_i^\dagger \bar{b}_j + \sum_i U_B n_{\bar{b}_i} n_{\bar{b}_i}. \quad (9)$$

III. NUMERICAL RESULTS FOR THE s -WAVE CASE

The system of equations (5)-(7) can be readily solved to yield the transition temperature T_c for the Leggett-BCS state and with variable t/U and filling factors. We, again, stress that there is an important difference [6] between the BEC limit in a gas and on a lattice. For the latter the transition temperature becomes zero at arbitrarily large attractive interactions. This is associated with the fact that the effective mass of the pair is infinite; pairs cannot hop without an intermediate unbinding which becomes prohibitively costly at large attraction. Very early on [6] it was anticipated that T_c would vary as $t^2/|U|$ in the deep BEC. We emphasize here that the validity of the scaling, $T_c \propto t^2/|U|$, requires minimally that the fermionic chemical potential μ be negative, i.e., the system must be in the bosonic regime. Indeed, as in earlier work [35] we find this dependence for T_c (but only) in the low density limit.

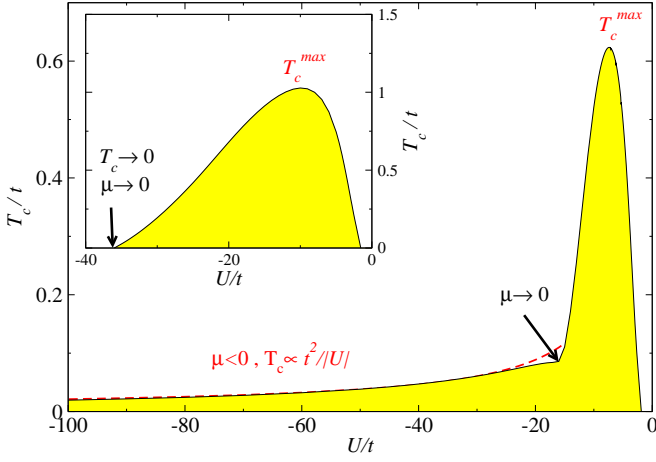


Figure 1: (Color online) T_c curve for s -wave pairing on a 3D lattice for $n = 0.3$ (black solid line). The tail is fitted to the functional form $t^2/|U|$ (red dash line). Inset: T_c curve for $n = 0.7$.

Figure 1 presents plots of T_c as a function of U/t at $n = 0.3$ and $n = 0.7$ (inset). For the first case, at low filling, T_c has a maximum in the regime where $\mu > 0$; once μ becomes negative we find a long tail with the expected $t^2/|U|$ dependence. This general behavior is consistent with earlier work [25, 35, 36]. It should be noted that, using rather different formalisms from that discussed here, others [20, 23] have reported this asymptotic t^2/U behavior, but have never correlated it with the bosonic regime, in the sense of requiring a negative μ . The plot in the inset emphasizes this point. At high n this figure shows that T_c vanishes right before the system crosses over into the bosonic regime. Also labeled on the plots for both cases is T_c^{max} , where the transition temperature reaches a maximum. As noted above, this maximum occurs at intermediate values of $|U|/t$ for all filling. As for the unitary limit in the case of homogeneous Fermi gases [11, 14], it occurs deep within the fermionic regime, where the chemical potential is still positive.

Figure 2 summarizes our phase diagram in the $U/t - n$ plane for the AHM with the shaded regimes indicating where the calculated T_c vanishes. Also indicated is the location of T_c^{max} as shown in Fig. 1 as a function of n . It is relatively constant in n , as observed by other groups [17, 18, 20]. Because of particle-hole symmetry at $n = 1$, here we only need to focus on the $n < 1$ half of the phase diagram.

We note that the upper boundary of the shaded region marking the breakdown of this superfluid phase is consistently near the $\mu = 0$ line (below which Cooper pairs start to behave like composite bosons), as might have been expected from the previous figure. Interestingly enough, this upper boundary (say, for $n \approx 0.5$) is not so far from the predicted values for $U/t = 35$ at which the superfluid-Mott insulator transition takes place for the BHM [43]. Note that for the BHM, U must be positive in order to stabilize Mott phases which derive from strong on-site inter-boson repulsion. Finally, we note that particle-hole symmetry near half filling effectively pins the chemical potential near the band center and the system has difficulty reaching the bosonic limit where the superfluid-

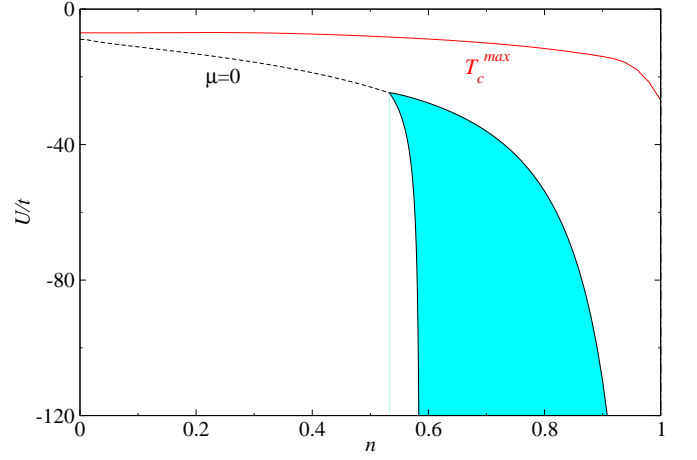


Figure 2: (Color online) $T \rightarrow 0$ phase diagram associated with the BCS-Leggett state for the AHM. The shaded region shows where superfluidity breaks down due to strong pairing fluctuations. The red line shows the trace of T_c^{max} in T_c plots as shown in Fig. 1. The black dashed line shows where $\mu = 0$, corresponding to the onset of a $t^2/|U|$ dependence in T_c , associated with low filling. At $n = 1$, there is an exact particle-hole symmetry.

ity is suppressed. As a result an increasingly more attractive interaction is required to arrive at the shaded region.

A key observation of our theory is that the character of the T_c curves changes at the point where μ changes sign. Another key observation is that, at large filling factors, the transition temperature *vanishes* near $\mu = 0$, when the system approaches the bosonic regime. This vanishing is associated with a localization of pairs, that is, a divergence of the pair effective mass. Physically this is not unexpected since we have seen the effective BEC Hamiltonian contains an inter-site repulsion of the same magnitude as the hopping term. It is this repulsion which inhibits pair hopping at large filling factors. Only in the low density limit can this inter-site repulsion be neglected, thereby leading to the conventional behavior, $T_c \propto t^2/|U|$. At larger filling, we find that this simple BCS-Leggett ground state will not support superfluidity in the $|U| \gg t$ limit.

We end this section by noting that while these calculations have been based on a theory which is compatible with the BCS-Leggett ground state, we believe our general conclusions will also apply if one were to address BCS-BEC crossover in a Hubbard model using alternative crossover schemes, for example, based on the NSR approach [6]. Below T_c , it has been shown [44] that the NSR scheme and related extensions treat the pairs in a weakly interacting fashion. This picture of weakly interacting “bosons” (at the level of Bogoliubov or Popov theory) cannot be appropriate for the Hubbard model near half filling and in the limit of strong attraction. Consequently, a proper self-consistent calculation of the transition temperature based on this starting point should show signs of the inadequacy of the NSR wave function ansatz, possibly through a vanishing of T_c such as we have found here.

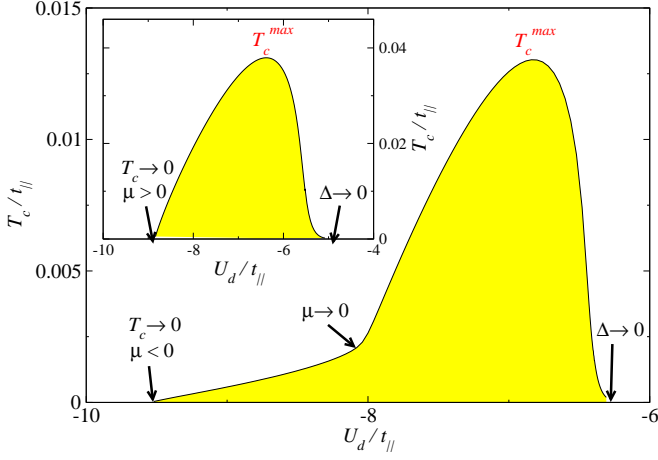


Figure 3: (Color online) Transition temperature T_c as a function of U_d/t_{\parallel} for d -wave pairing on a quasi-2D lattice for $n = 0.05$. At this low filling superfluidity can be sustained for some range of attractive interactions, even after μ becomes negative at moderately strong coupling. For strong enough attraction we find a strictly zero T_c . Inset: T_c curve for $n = 0.1$, for which T_c is nonzero only in the fermionic regime.

IV. NUMERICAL RESULTS FOR d -WAVE PAIRING

In this section we study the transition temperatures for the case of d -wave pairing. We can anticipate that as the system approaches stronger coupling, pair hopping will be greatly suppressed, just as for the s -wave case, and superfluidity will shut down. Indeed, because the d -wave pairs are extended over two lattice sites, the effects we saw for the s -wave case should be even more dramatic. Moreover, because there is no standard d -wave analogue of Eq. (8), it is not clear a priori whether the $\mu = 0$ point should reflect a qualitative change in the physics.

Figure 3 presents results for the d -wave transition temperature in a quasi-2D lattice for $n = 0.05$ and $n = 0.1$ (inset). A new feature emerges which is not present in the s -wave case. In the ground state, there is a threshold in $|U_d|/t$ above which weak coupling superfluidity is stable and below which it will not survive [40]. Just as for the s -wave case, at all fillings there is a maximum in the T_c curves which we refer to as T_c^{max} , inside the fermionic regime. Importantly, only at extremely low filling ($n < 0.1$) is T_c finite when μ becomes negative. Otherwise T_c vanishes for sufficiently strong attraction, but still within the fermionic regime, $\mu > 0$. In fact, even for those extremely low values of n , where one can pass into the bosonic regime, we find that T_c reaches zero for sufficiently large $|U_d|/t$. This shut-down of superfluidity is associated with a divergence in the pair mass, that is, with localization of the pairs, just as for the s -wave case.

Shown in Fig. 4 is the phase diagram in the $U_d - n$ plane for the d -wave case. In the light (gray) shaded region, there is no superfluid ground state associated with the BCS-Leggett $T = 0$ equations [5]. This is on the weak coupling side of the phase diagram. In the dark (cyan) shaded region, pairing fluctuations destroy superfluidity. This corresponds to the strong coupling

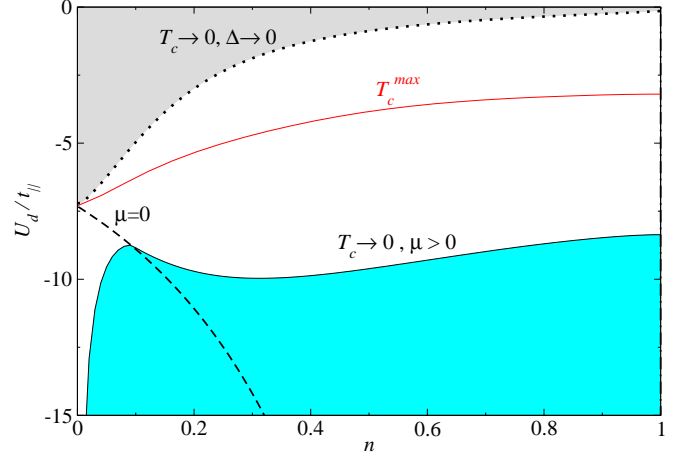


Figure 4: (Color online) $T \rightarrow 0$ phase diagram for fermions on a quasi-2D lattice with d -wave pairing symmetry. The lower (cyan) shaded regimes shows where superfluidity does not survive as $T \rightarrow 0$. The black dotted line indicates the threshold beyond which superfluidity becomes observable (i.e., in the unshaded regions) and the upper (gray) shaded regime corresponds to a normal phase. The red solid line shows the trace of T_c^{max} shown in Fig. 3. The black dash line indicates where $\mu = 0$.

side of the phase diagram, and arises because of inhibition of hopping.

It should be clear that in the d -wave case the regime where pairing fluctuations destroy superfluidity is much larger than its counterpart in the s -wave case. This reflects the fact that d -wave pairing involves nearest-neighbor sites. The finite size of the pairs (which cannot be less than the lattice constant) distinguishes them from the point-like composite bosons (of the s -wave case) and allows them to break and recombine with neighboring sites in complicated ways. In the very dilute limit we understand the behavior of Fig. 4 as follows. If a two-body-like bound pair state exists (i.e., when $\mu < 0$), the binding energy will be given by $E_b \approx -2\mu \sim \hbar^2/2m\xi^2$, where ξ is the pair size. Note that in a many-body system, the dimensionless quantity E_b/E_F must be large for a system to be in the BEC limit. The fact that the d -wave pair size ξ cannot be smaller than the lattice constant sets an upper bound for the binding energy.

Only in the dilute limit where the mean inter-particle distance becomes substantially larger than the d -wave pair size can one reach sufficiently large values of E_b/E_F to achieve a d -wave bosonic superfluid, principally because of the small value of n or E_F . In this low density regime, if we continue to increase the attraction (at very small fixed n) we again rapidly destabilize the superfluid phase. This is associated with the fact that increased attraction requires a larger and larger E_b (or equivalently smaller ξ), which eventually hits the limit set by the lattice constant.

Since the inter-particle distance $1/k_F$ in quasi-2D scales as $1/\sqrt{E_F} \sim n^{-1/2}$, with increasing n (at fixed attractive interaction) the relative binding energy E_b/E_F decreases very rapidly. As a result, $1/k_F$ soon becomes comparable to the pair size ξ , so that many-body effects strongly suppress the

mobility of the pairs. This eventually destroys the superfluid state.

Finally, as the density approaches half filling, additional effects arise from particle-hole symmetry. These tend to pin μ to its noninteracting value ($\approx 4t_{||}$). This explains why the chemical potential is high when T_c vanishes at densities close to half filling. In summary, despite the fact that the mean-field ground state equations have a superfluid solution, we find that with fluctuation effects included, this d -wave superfluidity (associated with the BCS-Leggett ground state) has difficulty becoming established once the attractive interaction becomes moderately strong.

V. LOCAL PAIR STATE (LPS) WAVE FUNCTION AND BCS-LPS TRANSITION

A. The breakdown of the BCS-Leggett state in the $|U| \gg t$ limit

We have emphasized that the shaded region in Fig. 2 is associated with the breakdown of the BCS-Leggett form of superfluidity. It is natural to ask what is the nature of the phase inside the shaded region. We have in the past [25] characterized this state as “insulating” on the basis of the general “rule” that a bosonic system which is non-superfluid is generally localized. Moreover, the onset of the shaded region that we find marks the onset of an infinite pair mass which is consistent with localized bosons. It has been argued [45] that an insulating phase for both fermions and bosons, if it corresponds to a finite excitation gap, is only possible when the filling is commensurate. One way to get around these arguments (which allow insulating phases away from commensurability) is to introduce phase separation which we do not contemplate here. It may also be that localized pair states with a “localization gap” arising from many body effects, (not disorder), cannot be ruled out. Finally, one may also consider other forms of superfluid phases which may be more stable than the BCS-Leggett form, although they need not evolve continuously from the BCS state. Indeed, based on a study of the true Bose case [39] there is a suggestion that the ground state might well be a superfluid whenever the nearest-neighbor repulsive term is smaller than twice the hopping coefficient.

We observe that when the on-site attraction is strong, fermions are expected to form local pairs and one might anticipate that a better ground state for the superfluid phase is one where a given site either has precisely zero ($n_i = 0$) or precisely 2 fermions. Singly occupied sites are unfavorable, although they do serve as opportunities for virtual hopping. It is convenient in what follows to count the number of bosons which correspond to 1/2 of the fermion number. Due to the particle-hole symmetry about $n_b = 1/2$, we restrict consideration to $0 < n_b < (1/2)$ where $n_b = \sum_i \langle n_{b_i} \rangle / N$ is the filling factor of pairs.

Following earlier work [28], we contemplate a new ground state

$$|LPS\rangle = \prod_i (\sqrt{1-n_b} + \sqrt{n_b} b_i^\dagger) |0\rangle. \quad (10)$$

An analogous wave function was discussed for bosonic systems [38]. We stress that the correct pair commutation relation $[b_i, b_i^\dagger] = 1 - 2n_{b_i}$ should be used. The ground state energy for any $0 < n_b \leq (1/2)$ is $\langle LPS | H_{eff} | LPS \rangle = Jz n_b (2n_b - 1)N$. Here z is the number of nearest neighbors. Following [38] the zero-momentum-pair fraction is $\langle LPS | b_i^\dagger | LPS \rangle^2 / n_b = 1 - n_b$. Thus, when $n_b \rightarrow 0$ nearly all pairs are in the zero-momentum condensate.

In this LPS state, near half filling, roughly half of the pairs at $T = 0$ have finite momentum. Note that this many body wave function is associated with a macroscopic occupation of the lowest effective single particle energy level, but that the effective single particle levels need not be eigenstates of the non-interacting system. Thus the ground state in question (for the strongly correlated case) is not associated with $(\mathbf{k}, -\mathbf{k})$ pairing. To see this in more detail, we rewrite the LPS state in momentum space

$$\begin{aligned} |LPS\rangle &= \prod_i (\sqrt{1-n_b} + \sqrt{n_b} c_{i\uparrow}^\dagger c_{i\downarrow}^\dagger) |0\rangle \\ &= \prod_i (\sqrt{1-n_b} + \sqrt{n_b} \sum_{\mathbf{p}, \mathbf{q}} c_{\mathbf{p}\uparrow}^\dagger c_{\mathbf{q}\downarrow}^\dagger e^{-i(\mathbf{p}+\mathbf{q}) \cdot \mathbf{R}_i}) |0\rangle. \end{aligned} \quad (11)$$

Here \mathbf{R}_i denotes the position vector of the i -th site. From this expression one sees that when n_b is finite, both finite momentum Cooper pairs $c_{\mathbf{k}\uparrow}^\dagger c_{-\mathbf{k}+\mathbf{q}\downarrow}^\dagger$ and higher order terms such as $c_{\mathbf{k}_1\uparrow}^\dagger c_{\mathbf{k}_2\uparrow}^\dagger c_{\mathbf{k}_3\downarrow}^\dagger c_{\mathbf{k}_4\downarrow}^\dagger$ are important. The presence of these finite momentum condensed pairs may relate to the general issue of condensate fragmentation [46] which occurs in the presence of degenerate ground states. The degeneracy of the strict atomic limit $|U|/t \rightarrow \infty$ is partially lifted when weak tunneling is included, but it appears that a more natural description of the superfluid phase should be one which abandons the $(\mathbf{k}, -\mathbf{k})$ pairing of the BCS-Leggett phase.

We note that at low filling, one might expect that since the nearest-neighbor repulsion is negligible this LPS ground state may not be very different from the usual BCS-Leggett state. The equivalence is straightforward to establish. For $n_b \ll 1$,

$$\begin{aligned} |LPS\rangle &= \prod_i (\sqrt{1-n_b} + \sqrt{n_b} b_i^\dagger) |0\rangle \\ &\approx (1 + \sqrt{n_b} \sum_{\mathbf{k}} c_{\mathbf{k}\uparrow}^\dagger c_{-\mathbf{k}\downarrow}^\dagger) |0\rangle \\ &\approx \prod_{\mathbf{k}} (\sqrt{1-n_b} + \sqrt{n_b} c_{\mathbf{k}\uparrow}^\dagger c_{-\mathbf{k}\downarrow}^\dagger) |0\rangle. \end{aligned} \quad (12)$$

Here $\sum_i b_i^\dagger = \sum_i c_{i\uparrow}^\dagger c_{i\downarrow}^\dagger = \sum_{\mathbf{k}} c_{\mathbf{k}\uparrow}^\dagger c_{-\mathbf{k}\downarrow}^\dagger$. When $n_b \rightarrow 0$, the BCS number equation $n = 2n_b = 2 \sum_{\mathbf{k}} v_{\mathbf{k}}^2$ and the normalization condition $u_{\mathbf{k}}^2 + v_{\mathbf{k}}^2 = 1$ lead to $u_{\mathbf{k}} \approx \sqrt{1-n_b}$ and $v_{\mathbf{k}} \approx \sqrt{n_b}$. As expected, the states $|LPS\rangle$ and $|BCS\rangle$ are equivalent in the $|U| \gg t$ provided we consider the $n \rightarrow 0$ limit. This is consistent with our earlier numerical results which show that there is no breakdown of superfluidity at any strong attraction in the BCS-Leggett phase provided the filling is low. For small n , the BCS wave function captures the main features of the AHM in the two limits $|U|/t \ll 1$ and $|U|/t \gg 1$ and it should be appropriate for describing the crossover behavior of the AHM for any $|U|/t$. This

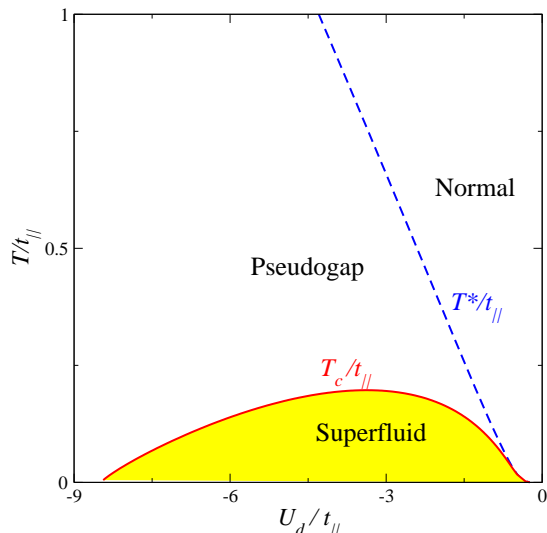


Figure 5: Phase diagram for d -wave pairing in a quasi-2D square lattice at $n = 0.9$ (near half filling). Pairs emerge below T^* but superfluidity only exists in the shaded regime. While the horizontal axis represents the strength of the attractive interaction, one may make contact with the cuprate phase diagram as shown in Fig. 7 of Ref. [8] by noting that the more underdoped the system the larger is T^* . Thus, one may view the hole doping concentration $x = 1 - n$ as a means of parameterizing the pairing attraction. In this way, there are some important similarities with the cuprates.

is no longer the case near half filling in the strongly attractive regime. The BCS-Leggett wavefunction does not capture the physics associated with strong inter-boson interactions, thereby leading us to contemplate an alternate superfluid phase, such as that associated with the LPS wavefunction. One might speculate that since the BCS-Leggett ground state and the LPS ground state describe different types of superfluids for very different limits, a quantum phase transition may occur when $|U|/t$ is tuned between these two limits. We speculate that the onset of this quantum phase transition can be loosely associated with the boundary curve for the shaded region in Fig. 2.

VI. EXPERIMENTAL IMPLICATIONS

A. Implications for High Temperature Superconductors

While there is an extensive literature [8, 9, 10] which argues that high T_c superconductivity can be “explained” by the repulsive Hubbard model, evidence that supports this point of view mainly comes from quantum Monte Carlo simulation or numerical study using a density matrix renormalization group method on a very small (e.g., 8×16) two dimensional lattice. Here we want to address what we can learn about the cuprates from the AHM. The phase diagram associated with the attractive Hubbard case, importantly, extended to d -wave pairing, is shown in Fig. 5 for the case of $n = 0.9$, which is appropriate for the cuprates and corresponds to hole doping concentration

$x = 1 - n = 0.1$. The behavior of the transition temperature was discussed in Sec. IV. Here we add an additional plot of T^* which corresponds to the pairing onset temperature. This is estimated by solving the standard mean field equations at $\Delta = 0$.

We stress at the outset that the BCS-BEC crossover scenario neither requires nor contains detailed microscopic information about the pairing mechanism. (More quantitative fits of this phase diagram to that of the cuprates have been presented in the literature [47]). Nevertheless, this phase diagram can be generically compared to that of the cuprates (see, e.g., Fig. 7 of Ref. [8]) without any detailed fits when we exploit the fact that (in the cuprate data) as x decreases, T^* increases. The more underdoped the system the larger is T^* . Thus, to make progress we may view the hole doping concentration x as a means of tuning the size of the pairing attraction. When T^* is matched to the experimental pseudogap onset temperature, the d -wave transition temperature displays a maximum as in the inset of Fig. 3, just as seen experimentally at the optimal doping. Importantly, one sees that when the attraction gets sufficiently strong superfluidity is shut down. Finally, we note that at the lower values for T^* (that is, in the overdoped regime), the superfluid phase in the cuprates is well described by d -wave BCS theory and the pseudogap is negligible. Thus the end-point for superconductivity at the lower critical doping in the cuprates may well be related to the break-down of BCS-BEC crossover which we have been discussing in this paper. It should be stressed, however, that this disappearance of the d -wave superfluid phase occurs well before one reaches the BEC limit. Indeed Fig. 4 shows clearly that the fermionic chemical potential is clearly positive (and large) when T_c vanishes at high fermion density. This is an important issue vis a vis the cuprates, since it is clear that these systems have a large positive fermionic chemical potential μ and are thus far from the bosonic regime.

A very important issue in high temperature superconductors, which has not been resolved experimentally, is a determination of the nature of that phase between a vanishing T_c and a large T^* at very low doping concentrations where superconductivity disappears. All that is certain is that it corresponds to an insulating state [8, 11] in the sense that the resistivity appears to increase with decreasing temperature. It should, in summary be clear that, although there may be differences associated with long range Coulomb effects which may, for example lead to phase separation [48], studies of attractive interactions on optical lattices have the potential for elucidating important issues in the high T_c cuprates.

B. Experiments on Optical Lattices

In this section we discuss possible experiments to observe BEC-BCS crossover on lattices in the specific context of the AHM. It is not at all straightforward to set up this fermionic one-band model and to avoid introducing either multi-band effects or direct boson-boson hopping. It should be stressed that on lattices, BEC-BCS crossover need not rely on a Feshbach resonance tuning of the attractive interaction alone. Rather, to

simulate the AHM, as shown in Refs. [3, 23, 49], the on-site attraction U and the hopping coefficient t are simultaneously tuned and are, thus, not independent. They can generally be controlled by varying the lattice potential depth V_0 as well as the s -wave scattering length a_s (of a Fermi gas in the absence of lattice potentials). It is conventional to define the recoil energy as $E_R \equiv \hbar^2/(2m\lambda^2)$, where λ is the wavelength of the laser used to generate the lattice potential and the lattice spacing is $d = \lambda/2$. Importantly, when $V_0 \gg E_R$ and $d \gg |a_s|$, it can be shown that the one-band Hubbard model emerges with $t = (2/\sqrt{\pi})E_R\xi^3e^{-2\xi^2}$ and $U = \pi E_R(a_s/d)\xi^3$, where $\xi = (V_0/E_R)^{1/4}$.

In the regime $a_s \geq d$ both multi-band effects and additional terms in the Hamiltonian such as density-assisted hopping terms become important [23]. Here the Hamiltonian can no longer be associated with the AHM. BCS-BEC crossover can readily occur in this limit without the interruption we have found in our Hubbard calculations. Indeed, when a Fermi gas is in the strongly attractive regime (the BEC side of a Feshbach resonance) in the absence of any lattice potential, fermions form pairs with true binding energies ($\sim \hbar^2/2ma_s^2$), and pairs repel each other with an effective scattering length $0.6a_s$ [50]. These two-body effects are robust when an optical lattice is then “switched on”. In this way a BEC limit can be readily established. More specifically, one starts with a Fermi gas in the deep BEC regime (satisfying $a_s \ll d$ when the lattice potential is turned off), and then increases the lattice depth. Importantly, the system can be described by a Bose Hubbard model with infinite on-site repulsion. In this case the two-body binding energy will dominate the on-site attractive potential of fermions. There is no effective nearest-neighbor repulsion (found in the BEC of fermion pairs) because the true binding energy of pairs prevents the presence of unpaired fermions and therefore eliminates these virtual processes. It should be noted that the first generation experiments from MIT on optical lattices [2] were performed making use of a Feshbach resonance so that before the optical lattice was established, the system was near unitarity. Again, these experiments should not be considered as simulating the one-band AHM. Rather they pertain to a model Hamiltonian which is clearly different from the fermion Hubbard model. We have argued in this paper, as claimed elsewhere [28], that this attractive fermion Hubbard model may have relevance to high temperature superconductors.

From the present perspective, based on the AHM, there are a variety of important experiments yet to be done. Among these is to see if one can find the predicted breakdown of BCS-BEC crossover which may be associated with the transition to a new type of superfluid (The BCS-Leggett state to the LPS state) or to some other type of non-superfluid order. To do this we propose that the Fermi gas is first prepared in the weakly attractive regime (on the BCS side of resonance) satisfying $|a_s| \ll d$ and then the lattice potential is gradually increased to suppress hopping. As shown in Fig. 4 of Ref. [23], this is equivalent to increasing $|U|/t$ in the AHM when $a_s < 0$. As $|U|/t$ increases, a maximum in T_c should first be observed. Near half filling when $|U|/t$ is sufficiently large (as predicted by Fig. 2) a new type of ordering may appear or alternatively

(if the associated transition temperatures are sufficiently low) the system will be driven normal. It is quite likely, although it may be hard to verify, that the loss of superfluid order is to be associated with a quantum phase transition near half filling and when $|U| \gg t$.

VII. CONCLUSIONS

In this paper we have addressed a generalization of BCS-BEC crossover in atomic Fermi systems to include the presence of an optical lattice. Our specific interest is to address the AHM, and in the longer term, its d -wave generalization which have been argued to be relevant to high T_c superconductors. While there have been a number of numerical studies [17, 18] of the attractive Hubbard Hamiltonian, along with approaches based on dynamical mean field theory [20, 23], ours is a systematic study over all filling fractions and over the entire range of attractive interactions.

We have investigated the stability of the simplest type of superfluid phases which represent a natural generalization of BCS-BEC crossover which has been widely studied in the gas phases. We refer to the ground state wave function as the “BCS-Leggett” state and find that, even though the strict $T = 0$ mean-field equations suggest that superfluidity can occur everywhere, fluctuation effects lead to a vanishing T_c over an extended range near half filling and for moderately strong attraction. Thus, there is an interruption of BCS-BEC crossover which we explain from an analytic viewpoint. This interruption occurs very close to the regime where the fermionic chemical potential $\mu = 0$. It is a result of the system passing over into the regime where the standard t^2/U -expanded bosonic Hamiltonian (as an approximation to the AHM) becomes valid. In contrast with the weakly interacting bosons of the BCS-Leggett state (or of the NSR theory), here the bosonic degrees of freedom experience a strong inter-site repulsion. Importantly superfluidity in these specific (weak coupling) forms cannot be supported.

We posit an alternative superfluid phase which may be more appropriate at very strong attraction. These studies have been extended to the d -wave case as well. We stress that the resulting phase diagram has many features in common with that of the cuprates. In particular, at sufficiently strong attraction (as represented by a large value for the pairing onset temperature, called T^*), superfluidity is interrupted. This interruption of BCS-BEC crossover occurs while the system still has a rather large positive fermionic chemical potential, and hence is far from the BEC.

A central goal of this body of work is to make a case for future optical lattice experiments to simulate the AHM, first for the s -wave and ultimately for the d -wave case. It is our contention that in this way we have as much to learn about the cuprate superconductors, as from studies of the repulsive Hubbard model which has been conjectured to give rise to d -wave attraction.

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